LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049173.D
Acq On : 2 Jul 2021 18:51
Operator : CG/JU
Sample : M2904-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** COMP-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049173.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.126 | 9 | 15 | 24 | rBV2 | 60053 | 138175 | 5.77% | 1.179% |
| 2 | 3.208 | 25 | 29 | 35 | rVB | 22154 | 36477 | 1.52% | 0.311% |
| 3 | 5.164 | 357 | 362 | 371 | rBV3 | 15715 | 31039 | 1.30% | 0.265% |
| 4 | 5.640 | 434 | 443 | 454 | rBV | 616005 | 1032299 | 43.13% | 8.811% |
| 5 | 7.238 | 708 | 715 | 727 | rBV | 643640 | 1114145 | 46.55% | 9.509% |
| 6 | 8.084 | 852 | 859 | 868 | rBV | 122490 | 211864 | 8.85% | 1.808% |
| 7 | 9.254 | 1049 | 1058 | 1067 | rBV | 393003 | 708919 | 29.62% | 6.051% |
| 8 | 10.670 | 1292 | 1299 | 1307 | rBV4 | 25810 | 51005 | 2.13% | 0.435% |
| 9 | 10.905 | 1332 | 1339 | 1346 | rBV | 161663 | 294566 | 12.31% | 2.514% |
| 10 | 13.355 | 1748 | 1756 | 1765 | rBV | 980236 | 1561671 | 65.25% | 13.329% |
| 11 | 14.730 | 1982 | 1990 | 1999 | rVB | 296575 | 453725 | 18.96% | 3.873% |
| 12 | 16.216 | 2236 | 2243 | 2256 | rBV | 1025858 | 1606480 | 67.13% | 13.711% |
| 13 | 17.479 | 2451 | 2458 | 2464 | rBV | 365007 | 583626 | 24.39% | 4.981% |
| 14 | 20.082 | 2895 | 2901 | 2908 | rBV | 1788029 | 2393211 | 100.00% | 20.426% |
| 15 | 21.392 | 3119 | 3124 | 3133 | rBV5 | 59093 | 109933 | 4.59% | 0.938% |
| 16 | 21.763 | 3180 | 3187 | 3197 | rBV | 366735 | 615401 | 25.71% | 5.252% |
| 17 | 23.496 | 3476 | 3482 | 3488 | rVB2 | 41713 | 79857 | 3.34% | 0.682% |
| 18 | 24.125 | 3585 | 3589 | 3596 | rVB7 | 14158 | 29784 | 1.24% | 0.254% |
| 19 | 25.065 | 3740 | 3749 | 3767 | rVB2 | 210321 | 664323 | 27.76% | 5.670% |

Sum of corrected areas: 11716500

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Misc :
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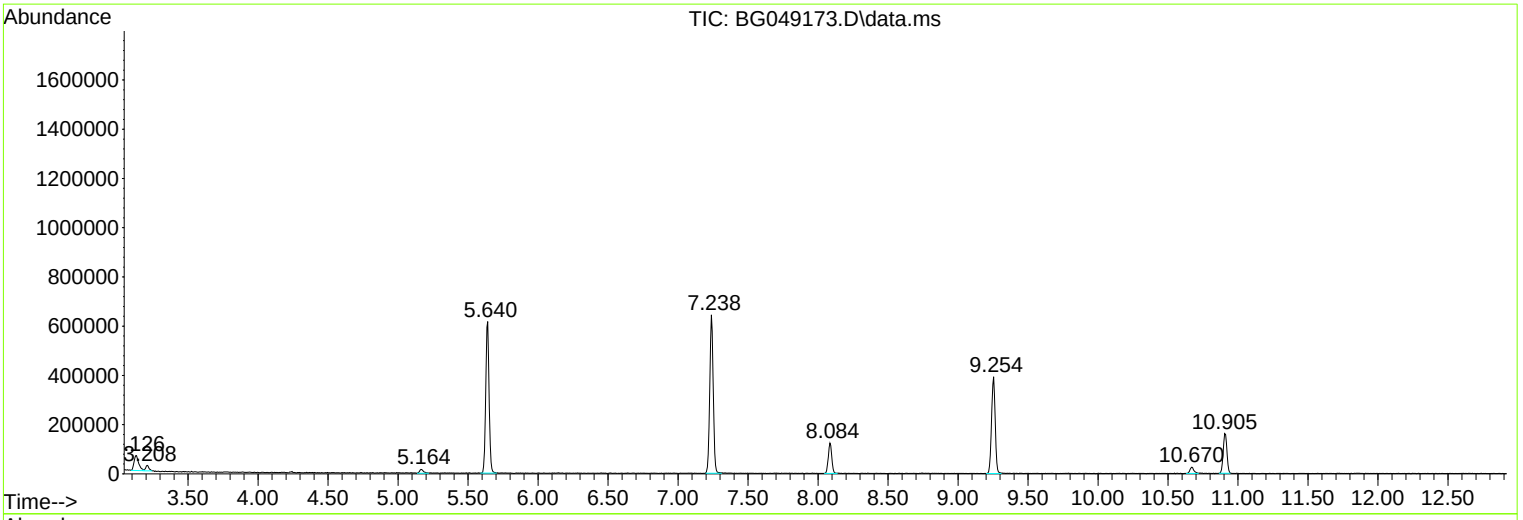
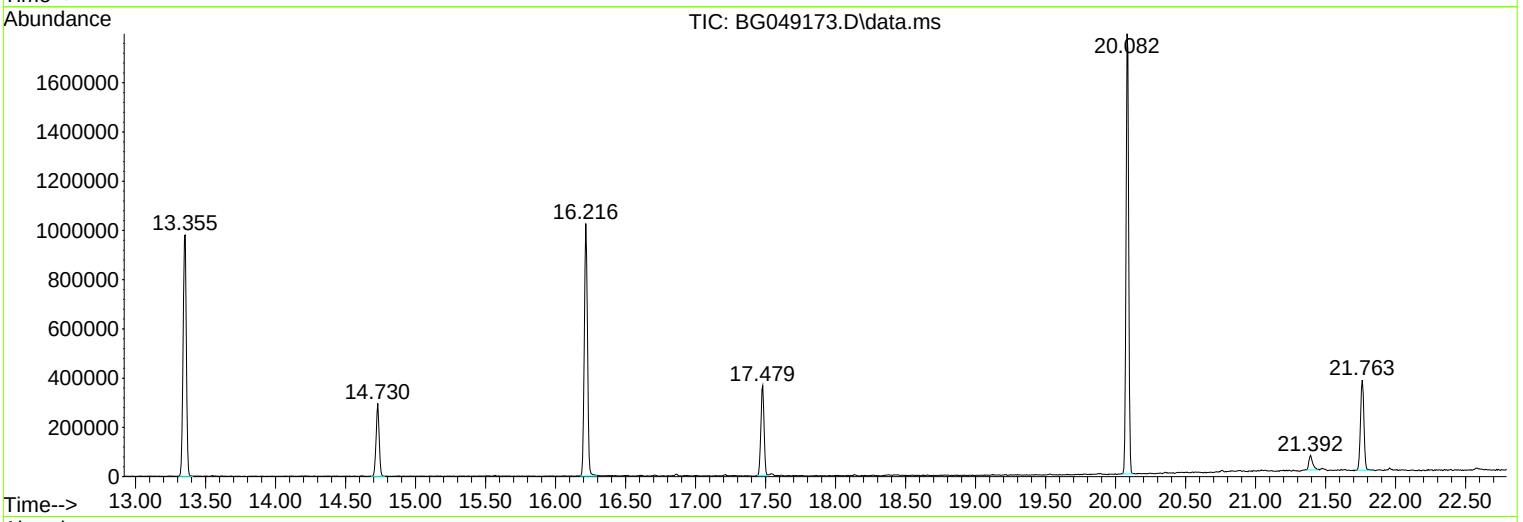
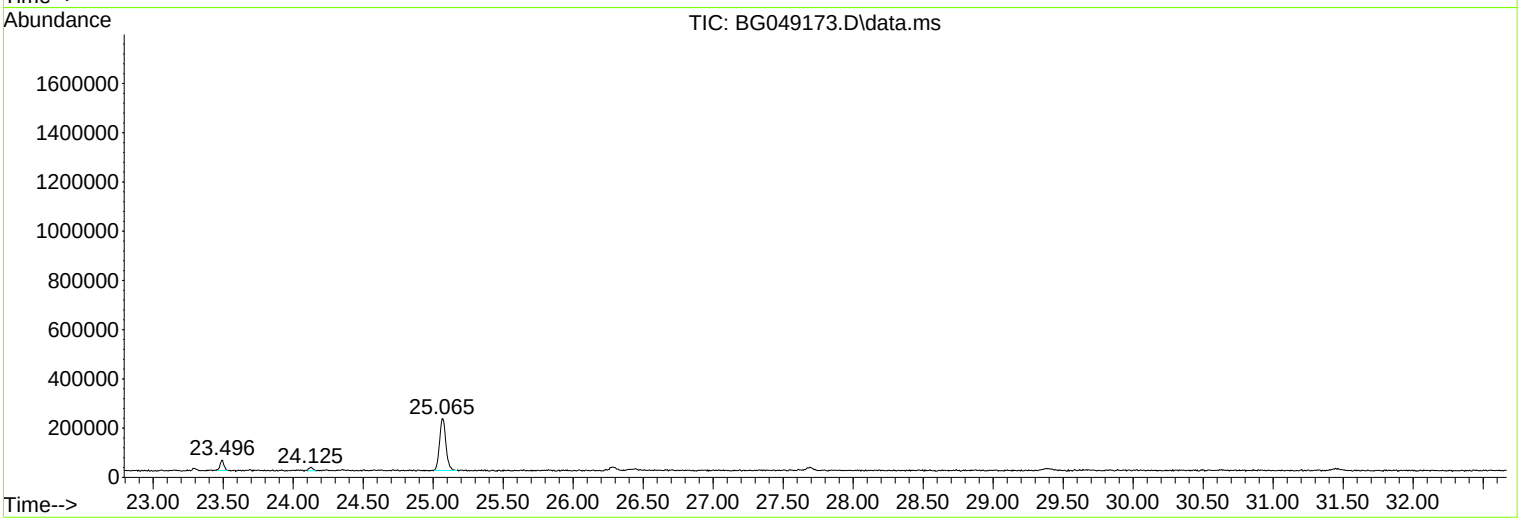
**Instrument :**
BNA_G
**ClientSampleId :**
COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

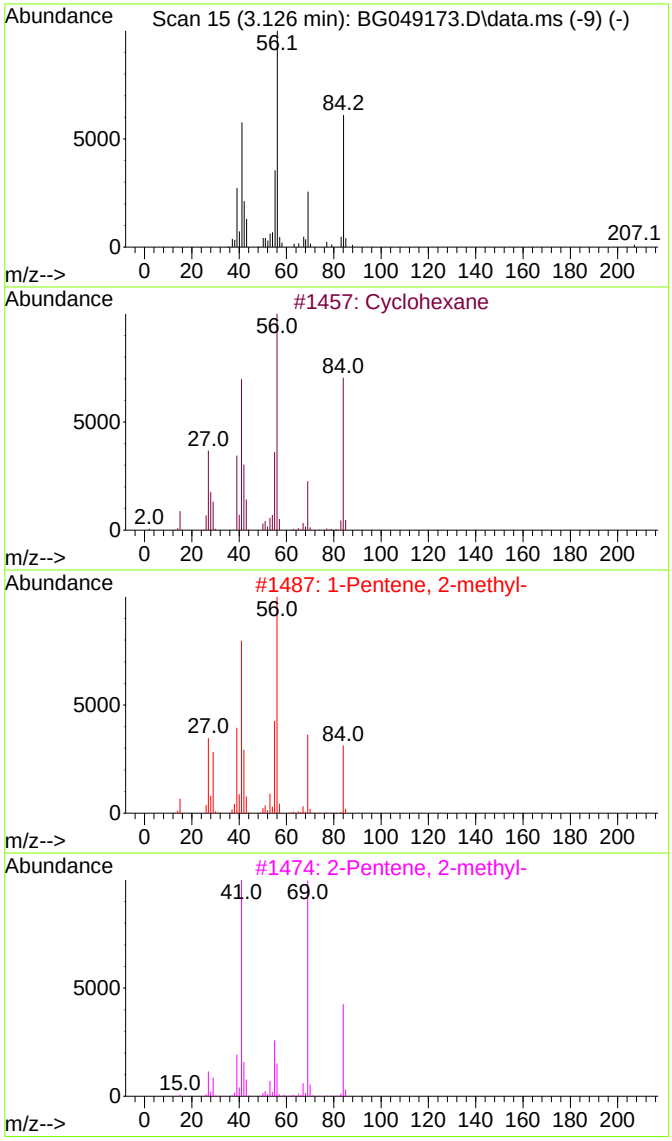
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

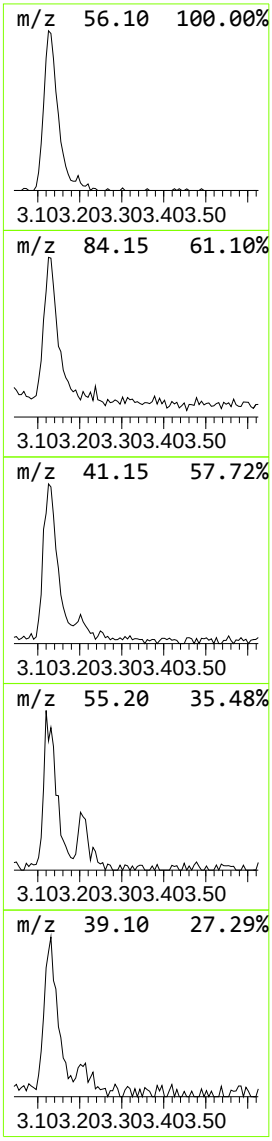
**********

Peak Number 1 Cyclohexane Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.126 | 13.04 ng | 138175 | 1,4-Dichlorobenzene-d4 | 8.090 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane | 84 | C6H12 | 000110-82-7 | 90 |
| 2 | 1-Pentene, 2-methyl- | 84 | C6H12 | 000763-29-1 | 72 |
| 3 | 2-Pentene, 2-methyl- | 84 | C6H12 | 000625-27-4 | 43 |
| 4 | Cyclobutane, ethyl- | 84 | C6H12 | 004806-61-5 | 43 |
| 5 | Cyclobutanecarbonitrile, 3,3-dim... | 109 | C7H11N | 053783-86-1 | 38 |



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Operator : CG/JU
Sample : M2904-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

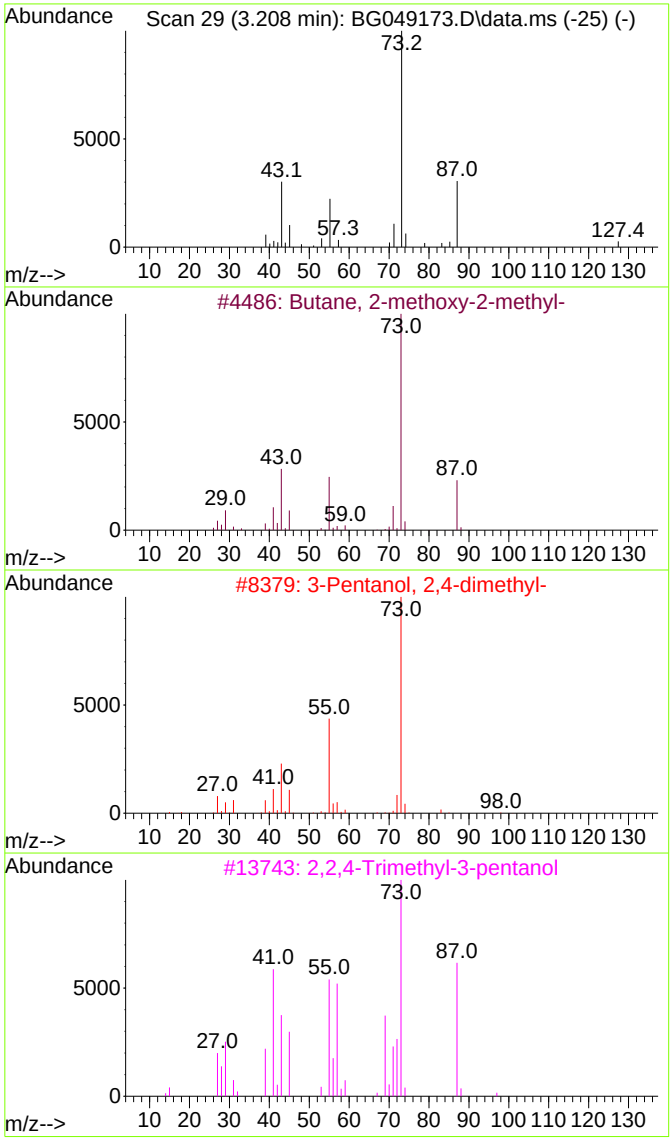
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

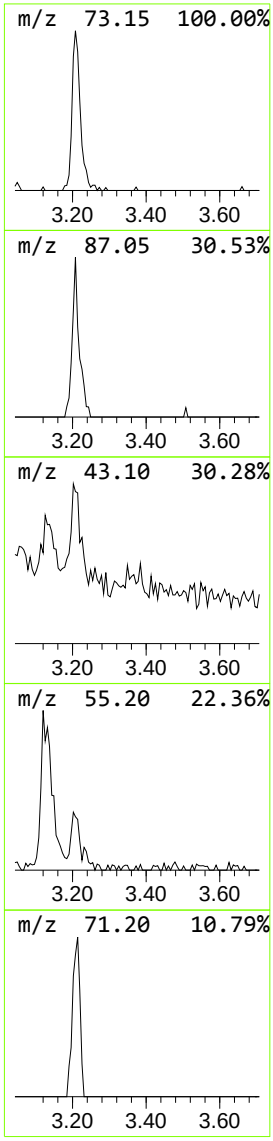
**********

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.208 | 3.44 ng | 36477 | 1,4-Dichlorobenzene-d4 | 8.090 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 72 |
| 2 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 17 |
| 3 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 9 |
| 4 | 1,3-Dioxolane, 2-(1-methylethyl)- | 116 | C6H12O2 | 000822-83-3 | 9 |
| 5 | Isopropyl 5,11-dihydroxy-3,7,11-... | 314 | C18H34O4 | 1000223-34-1 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049173.D
Acq On : 2 Jul 2021 18:51
Operator : CG/JU
Sample : M2904-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMP-3

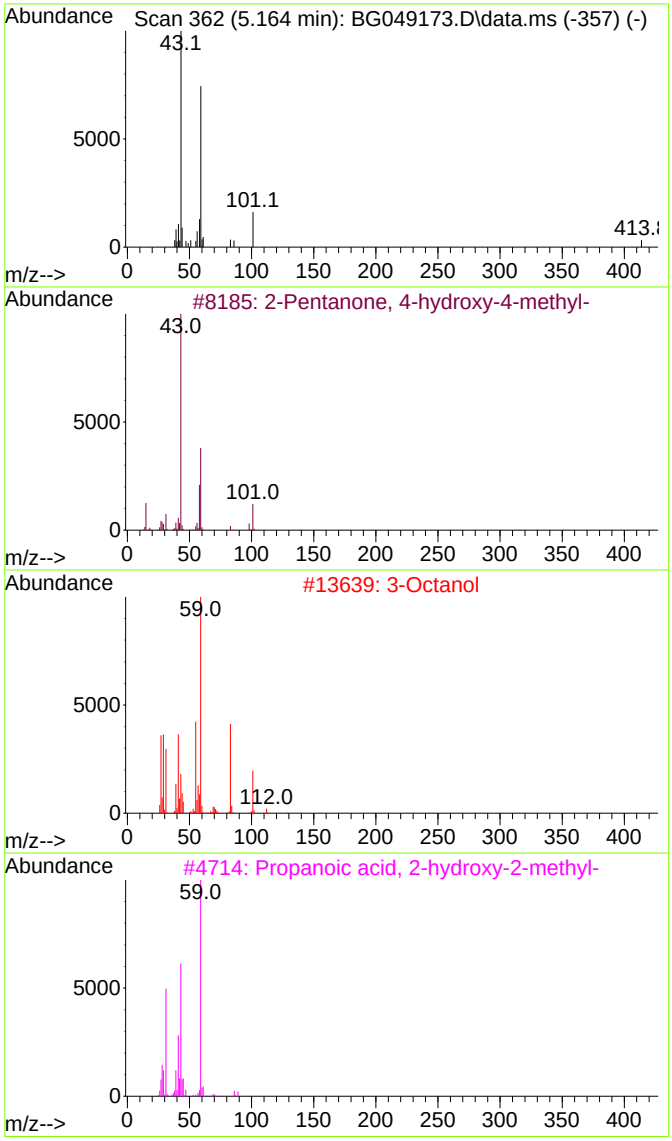
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

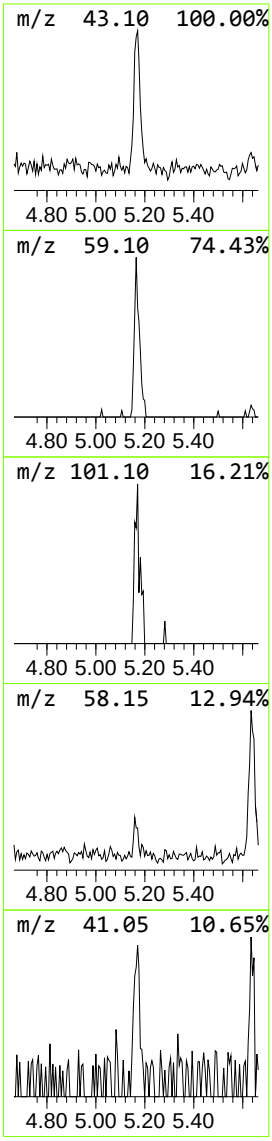
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.164 | 2.93 ng | 31039 | 1,4-Dichlorobenzene-d4 | 8.090 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 3-Octanol | 130 | C8H18O | 000589-98-0 | 45 |
| 3 | Propanoic acid, 2-hydroxy-2-methyl- | 104 | C4H8O3 | 000594-61-6 | 38 |
| 4 | 2-[2-(2-Methoxyethoxy)ethoxy]eth... | 236 | C10H24O4Si | 1000352-07-3 | 38 |
| 5 | 1,1-Dimethyl-2-[2-methyl-1-(meth... | 174 | C8H18N2O2 | 097812-29-8 | 38 |



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Operator : CG/JU
Sample : M2904-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** COMP-3

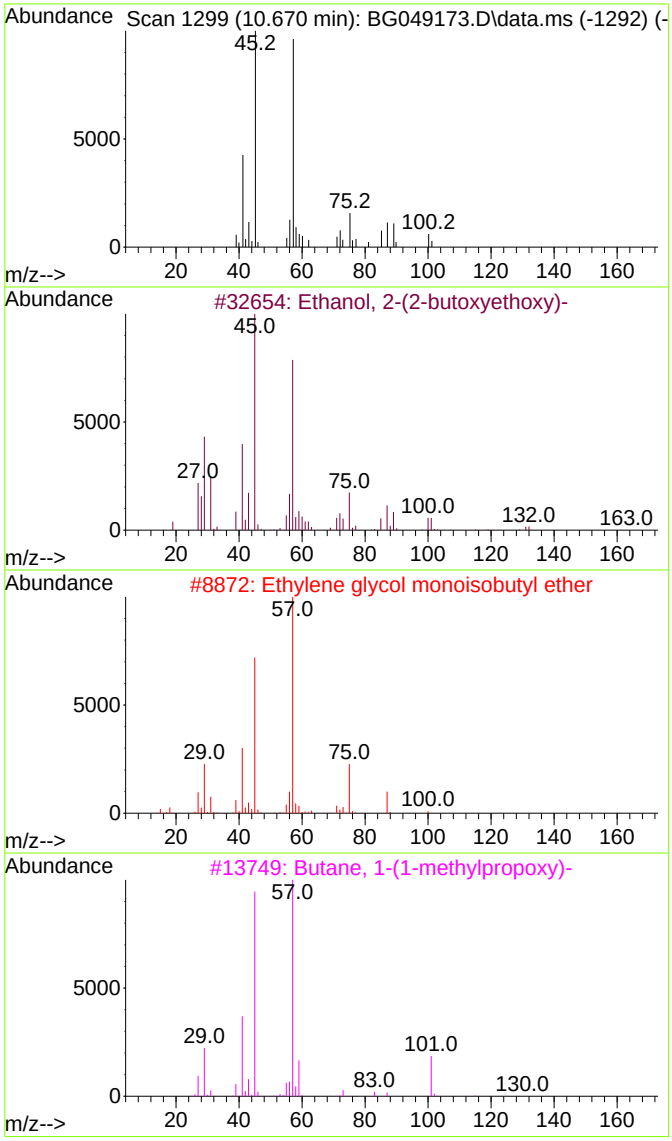
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

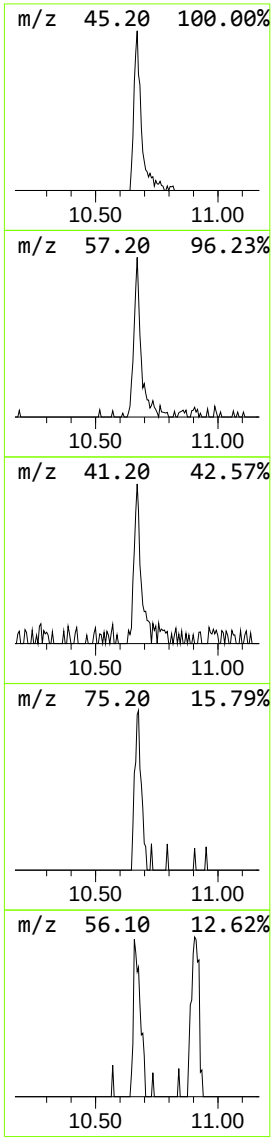
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.670 | 3.46 ng | 51005 | Naphthalene-d8 | 10.905 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 64 |
| 2 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 59 |
| 3 | Butane, 1-(1-methylpropoxy)- | 130 | C8H18O | 000999-65-5 | 53 |
| 4 | Methoxyacetic acid, 2-butyl ester | 146 | C7H14O3 | 070159-90-9 | 50 |
| 5 | Ethanol, 2-[2-(2-butoxyethoxy)et... | 206 | C10H22O4 | 000143-22-6 | 45 |



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Sample : M2904-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMP-3

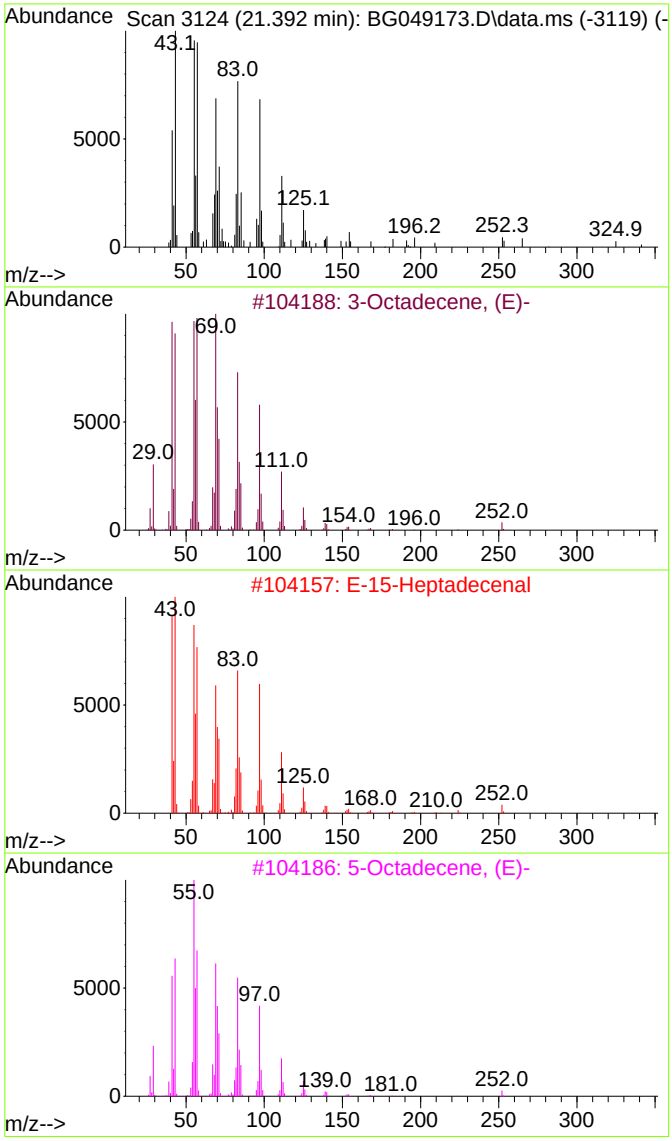
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

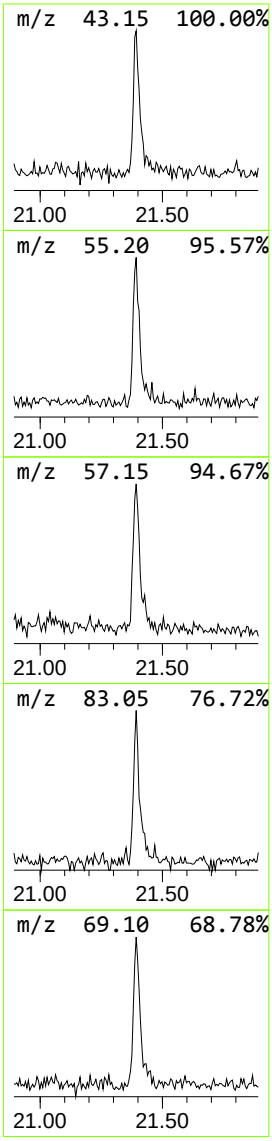
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 3-Octadecene, (E)- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.392 | 3.57 ng | 109933 | Chrysene-d12 | 21.763 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Octadecene, (E)- | 252 | C18H36 | 007206-19-1 | 94 |
| 2 | E-15-Heptadecenal | 252 | C17H32O | 1000130-97-9 | 94 |
| 3 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 94 |
| 4 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 94 |
| 5 | 9-Octadecene, (E)- | 252 | C18H36 | 007206-25-9 | 93 |



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Sample : M2904-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
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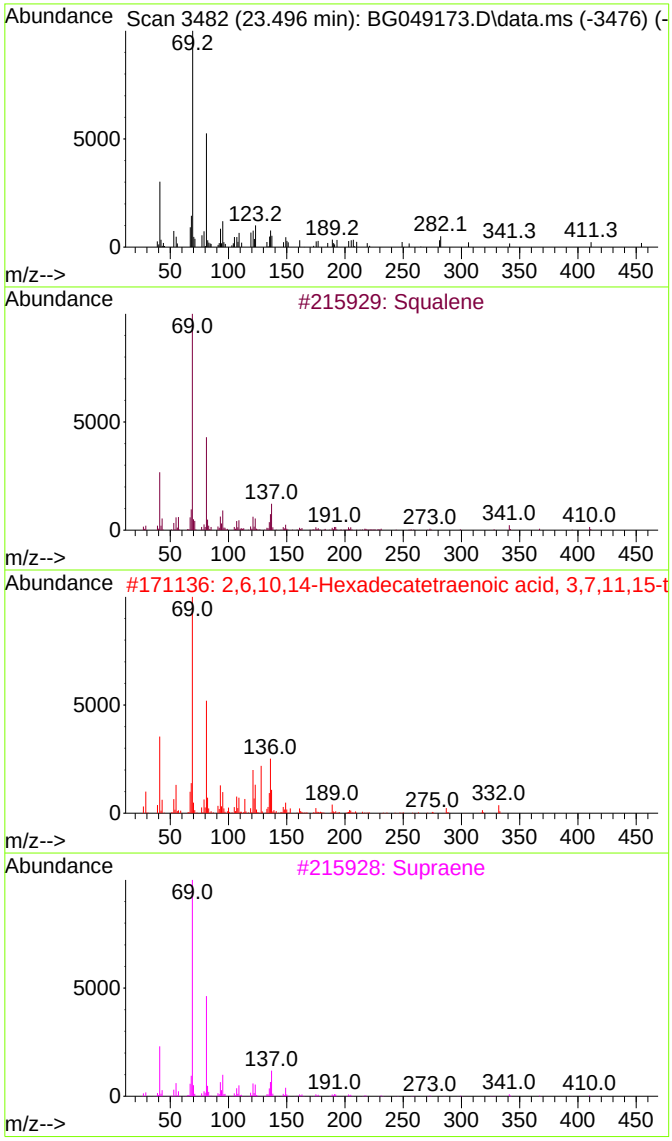
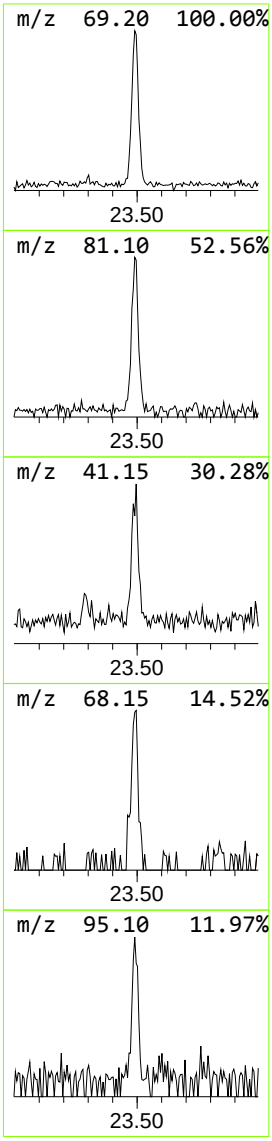
**********

Peak Number 6 Squalene Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.496 | 2.40 ng | 79857 | Perylene-d12 | 25.065 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 64 |
| 2 | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 64 |
| 3 | Supraene | 410 | C30H50 | 007683-64-9 | 64 |
| 4 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 50 |
| 5 | 2-Butenoic acid, 4-nitrophenyl e... | 207 | C10H9NO4 | 035665-90-8 | 50 |



Tentatively Identified Compound (LSC) summary

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Misc :
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TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Cyclohexane | 3.126 | 13.0 | ng | 138175 | 1 | 8.090 | 211864 | 20.0 |
| Butane, 2-metho... | 3.208 | 3.4 | ng | 36477 | 1 | 8.090 | 211864 | 20.0 |
| 2-Pentanone, 4-... | 5.164 | 2.9 | ng | 31039 | 1 | 8.090 | 211864 | 20.0 |
| Ethanol, 2-(2-b... | 10.670 | 3.5 | ng | 51005 | 2 | 10.905 | 294566 | 20.0 |
| 3-Octadecene, (E)- | 21.392 | 3.6 | ng | 109933 | 5 | 21.763 | 615401 | 20.0 |
| Squalene | 23.496 | 2.4 | ng | 79857 | 6 | 25.065 | 664323 | 20.0 |